# Dodecanoic acid octadeca-9,12,15-trienyl ester, Z,Z,Z

**Inchi:** InChI=1S/C30H54O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-21-23-25-27-29-32-30(31)28-

**InchiKey:** BGGKKRZHEDCMBO-QXYPMXJESA-N

**Formula:** C30H54O2

**SMILES:** CCC=CCC=CCC=CCCCCCCCCCOC(=O)CCCCCCCCCCC

**Mol. weight [g/mol]:** 446.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 208.46 | kJ/mol | Joback Method |
| hf | -555.67 | kJ/mol | Joback Method |
| hfus | 76.85 | kJ/mol | Joback Method |
| hvap | 91.40 | kJ/mol | Joback Method |
| log10ws | -10.80 | | Crippen Method |
| logp | 10.040 | | Crippen Method |
| mcvol | 428.100 | ml/mol | McGowan Method |
| pc | 658.81 | kPa | Joback Method |
| rinpol | 3124.42 | | NIST Webbook |
| tb | 974.57 | K | Joback Method |
| tc | 1201.38 | K | Joback Method |
| tf | 484.78 | K | Joback Method |
| vc | 1.679 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1466.37 | J/mol×K | 974.57 | Joback Method |
| cpg | 1490.62 | J/mol×K | 1012.37 | Joback Method |
| cpg | 1513.61 | J/mol×K | 1050.17 | Joback Method |
| cpg | 1535.47 | J/mol×K | 1087.97 | Joback Method |
| cpg | 1556.35 | J/mol×K | 1125.77 | Joback Method |
| cpg | 1576.37 | J/mol×K | 1163.58 | Joback Method |
| cpg | 1595.68 | J/mol×K | 1201.38 | Joback Method |
| dvisc | 0.0003996 | Pa×s | 484.78 | Joback Method |
| dvisc | 0.0001440 | Pa×s | 566.41 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000671 | Pa×s | 648.04 | Joback Method |
| dvisc | 0.0000371 | Pa×s | 729.67 | Joback Method |
| dvisc | 0.0000231 | Pa×s | 811.31 | Joback Method |
| dvisc | 0.0000157 | Pa×s | 892.94 | Joback Method |
| dvisc | 0.0000114 | Pa×s | 974.57 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R437166&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume